

Quantum state sensitivity to initial conditions

Gonzalo Garcia de Polavieja*

Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, U.K.

Abstract

The different time-dependent distances of two arbitrarily close quantum or classical-statistical states to a third fixed state are shown to imply an experimentally relevant notion of state sensitivity to initial conditions. A quantitative classification scheme of quantum states by their sensitivity and instability in state space is given that reduces to the one performed by classical-mechanical Lyapunov exponents in the classical limit.

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*Electronic mail: gonzalo@rydberg.thchem.ox.ac.uk

Stimulated by the pioneering work of Peres [1,2] on state sensitivity to small changes in the Hamiltonian, several new developments have taken the study of quantum state sensitivity to the experimental realm. Schack and Caves [3] have analyzed the sensitivity to perturbations as the amount of information about a perturbing environment that is needed to keep entropy from increasing. Their approach links the study of quantum sensitivity to statistical mechanics and to quantum information theory. Recently, Gardiner *et al.* [4] have proposed a detailed experimental set-up of an ion trap to study quantum state sensitivity to changes in the Hamiltonian. A different approach has been taken by Ballentine and Zibin [5] that study the emergence of classical state sensitivity from quantum theory in computational time reversal. The difficulty of directly tackling the problem of quantum state sensitivity to initial conditions stems from the following reason. Classical sensitivity to initial conditions is made precise when measured by Lyapunov characteristic exponents [6]

$$\lambda_c(\mathbf{x}_0) = \lim_{d_c(0) \rightarrow 0} \lim_{t \rightarrow \infty} \frac{1}{t} \ln \left(\frac{d_c(\mathbf{x}_t, \mathbf{y}_t)}{d_c(\mathbf{x}_0, \mathbf{y}_0)} \right) \quad (1)$$

with $d_c(\mathbf{x}_t, \mathbf{y}_t)$ the Euclidean distance [7] between two phase space vectors \mathbf{x}_t and \mathbf{y}_t . There is classical sensitivity to initial conditions when $\lambda_c(\mathbf{x}_0) > 0$ and the trajectory starting at \mathbf{x}_0 is said to be unstable. A direct attempt to define the quantum analog of the classical Lyapunov characteristic exponent in (1) substitutes the phase space distance between two classical trajectories by the Hilbert-space \mathcal{H} distance between two close quantum vectors giving

$$\lambda_{\mathcal{H}}[|\psi(0)\rangle] = \lim_{d_{\mathcal{H}}(0) \rightarrow 0} \lim_{t \rightarrow \infty} \frac{1}{t} \ln \left(\frac{d_{\mathcal{H}}(|\psi(t)\rangle, |\varphi(t)\rangle)}{d_{\mathcal{H}}(|\psi(0)\rangle, |\varphi(0)\rangle)} \right) = 0, \quad (2)$$

a zero quantum Lyapunov exponent for all states as any two states do not separate at all with $d_{\mathcal{H}}(|\psi(t)\rangle, |\varphi(t)\rangle) \equiv \||\psi(t)\rangle - |\varphi(t)\rangle\| = \||\psi(0)\rangle - |\varphi(0)\rangle\|$ and $\|\cdot\| = \sqrt{\langle \cdot | \cdot \rangle}$. According to (2) all possible quantum states are stable and no sensitivity of quantum states to initial conditions can be found.

However, there are three strong objections against the use of $\lambda_{\mathcal{H}}$ as a measure of state sensitivity to initial conditions and instability. Firstly, the quantum mechanical state

space is the complex projective Hilbert space \mathbf{CP}^n that has a curvature not present in the complex Hilbert space \mathcal{H}_C^{n+1} . It is a nontrivial Kähler manifold with a symplectic form and an associated Riemannian metric [8]. Secondly, equation (2) is obtained by substituting the classical phase space trajectory distance in (1) by a quantum distance. This is not a mere technical error but a conceptual one as the closest classical object to a quantum state is a Liouville density, not a single trajectory [2,3,5]. Recall for example that in the classical limit the dynamical equation for the Wigner function or for the coherent state representation of the quantum density reduce to the Liouville equation [2]. A definition analogous to (2) for Liouville densities gives $\lambda_{\mathcal{L}}[\rho(0)] = 0$ with $d_{\mathcal{L}}(\rho_1(t), \rho_2(t)) \equiv \sqrt{\int dq dp \rho_1^{1/2}(q, p, t) \rho_2^{1/2}(q, p, t)} = d_{\mathcal{L}}(\rho_1(0), \rho_2(0))$ by Koopman's theorem. The fact that $\lambda_{\mathcal{L}}(\rho(t)) = 0$ for all possible Liouville densities tells us that we cannot know from (2) if quantum states have sensitivity as this type of measure for classical Liouville densities is insensitive to classical-mechanical instability. Thirdly, unlike the classical trajectory distance, $d_{\mathcal{H}}$ is a bounded metric, thus precluding the exponential divergence. In this paper we propose to overcome the above three objections in three steps to provide a working scheme to classify quantum and classical-statistical states by their sensitivity and instability in projective space \mathcal{P}^n . This sensitivity and instability are shown to be measurable by the different transition probabilities of two nearby states to a third fixed state.

Step 1. A classical density $\rho(x)$ can be mapped into a real Hilbert space \mathcal{H}_R^{n+1} by taking its square root, $\psi_c(x) \equiv \sqrt{\rho(x)}$. The expectation of a classical operator F is $\langle F \rangle = \langle F \psi_c^2 \rangle / \langle \psi_c^2 \rangle$, which means that the physical space is not \mathcal{H}_R^{n+1} but the space of equivalence classes obtained by identifying $\psi_c \sim \lambda \psi_c$ for any $\lambda \in \mathbf{R} - \{0\}$. This physical space is the real projective space \mathbf{RP}^n . Similarly, in quantum mechanics the true physical space is not the complex Hilbert space \mathcal{H}_C^{n+1} but the space of equivalent classes obtained by identification of vectors $\psi_Q \sim \lambda \psi_Q$ for any $\lambda \in \mathbf{C} - \{0\}$, the complex projective space \mathbf{CP}^n . Classical and quantum states in \mathcal{P}^n will be written as $\tilde{\psi}$. The distance between two points in \mathcal{P}^n (real or complex) can be defined as

$$d_{\mathcal{P}} [\tilde{\psi}_1, \tilde{\psi}_2] = 2 \arccos \left| \left\langle \frac{\psi_1}{\|\psi_1\|}, \frac{\psi_2}{\|\psi_2\|} \right\rangle \right|, \quad (3)$$

which is the length of the geodesic connecting the two points in \mathcal{P}^n as measured by the Fubini-Study metric [8,9].

Step 2. Now we are faced with the problem of finding relevant distances to characterize the motion of classical-statistical and quantum systems by their sensitivity and stability properties. According to the quantum expectation rule [2], the probability that a quantum state prepared in state $\tilde{\psi}_S$ will pass successfully the test for the state $\tilde{\psi}_R$ is $|\langle \tilde{\psi}_S | \tilde{\psi}_R \rangle|^2$. This shows that the distances of two arbitrarily close states $\tilde{\psi}_S$ and $\tilde{\psi}_S + \delta\tilde{\varphi}$ to a third fixed state $\tilde{\psi}_R$ are experimentally relevant as from (3) $|\langle \tilde{\psi}_S | \tilde{\psi}_R \rangle|^2 = \cos^2(d_{\mathcal{P}} [\tilde{\psi}_S, \tilde{\psi}_R] / 2)$ and similarly for $|\langle \tilde{\psi}_S + \delta\tilde{\varphi} | \tilde{\psi}_R \rangle|^2$. These distances $d_{\mathcal{P}} [\tilde{\psi}_S(t), \tilde{\psi}_R]$ and $d_{\mathcal{P}} [\tilde{\psi}_S(t) + \delta\tilde{\varphi}(t), \tilde{\psi}_R]$ are different and time-dependent and their difference is expected to behave differently in stable and unstable systems.

Step 3. The distance between two states in (3) is bounded, $d_{\mathcal{P}} \in [0, \pi]$, which obviously precludes exponential divergence. To understand how to study unstable systems in terms of a bounded metric we express the unbounded phase space Euclidean distance, $d_c \in [0, \infty)$, in terms of a bounded distance, say $d_c^b \in [0, \pi]$, that preserves the topology (d_c^b is 0 iff d_c is 0) as [10]

$$d_c^b(\mathbf{x}, \mathbf{y}) \equiv \pi d_c(\mathbf{x}, \mathbf{y}) / (1 + d_c(\mathbf{x}, \mathbf{y})) \quad (4)$$

The classical-mechanical Lyapunov exponent in (1) can then be expressed in terms of the classical bounded metric in (4) as

$$\lambda_c(\mathbf{x}_0) = \lim_{\Lambda_c(0) \rightarrow 0} \lim_{t \rightarrow \infty} \frac{1}{t} \ln (\Lambda_c(\mathbf{x}_t, \mathbf{y}_t) / \Lambda_c(\mathbf{x}_0, \mathbf{y}_0)). \quad (5)$$

with $\Lambda_c(\mathbf{x}, \mathbf{y})$ the *divergence* function that is the unbounded phase space distance expressed in terms of the bounded one as

$$\Lambda_c(\mathbf{x}, \mathbf{y}) \equiv d_c^b(\mathbf{x}, \mathbf{y}) / (\pi - d_c^b(\mathbf{x}, \mathbf{y})). \quad (6)$$

We are now ready to overcome the three objections to the definition in (2) and propose an analogue of the classical-mechanical Lyapunov exponent in \mathcal{P}^n (that we name \mathcal{P} -Lyapunov exponent). Let $\tilde{\psi}_S(t)$ and $\tilde{\psi}_S(t) + \delta\tilde{\varphi}(t)$ be two arbitrarily close system states and $\tilde{\psi}_R$ a reference state on the path $\tilde{\psi}_S(t)$, $\tilde{\psi}_R = \tilde{\psi}_S(\tau)$. The \mathcal{P} -Lyapunov exponent is obtained by the different distances of the two arbitrarily close system states to the reference point of the form

$$\lambda_{\mathcal{P}}^\infty [\tilde{\psi}_S(0)] = \lim_{\delta \rightarrow 0} \lim_{t \rightarrow \infty} \frac{1}{t} \ln \left| \frac{\Lambda [\tilde{\psi}_S(t)] - \Lambda [\tilde{\psi}_S(t) + \delta\tilde{\varphi}(t)]}{\Lambda [\tilde{\psi}_S(0)] - \Lambda [\tilde{\psi}_S(0) + \delta\tilde{\varphi}(0)]} \right| \quad (7)$$

with $\Lambda [\tilde{\psi}_S(t)]$ the *divergence* function for the distance between the system state $\tilde{\psi}_S(t)$ and the reference state $\tilde{\psi}_R$

$$\Lambda [\tilde{\psi}_S(t)] \equiv d_{\mathcal{P}} [\tilde{\psi}_R, \tilde{\psi}_S(t)] / (\pi - d_{\mathcal{P}} [\tilde{\psi}_R, \tilde{\psi}_S(t)]) \quad (8)$$

and $d_{\mathcal{P}}$ the bounded distance between states in (3). There is sensitivity to the initial condition $\tilde{\psi}_S(0)$ of degree $\lambda_{\mathcal{P}}^\infty$ when $\lambda_{\mathcal{P}}^\infty > 0$ and the path $\tilde{\psi}_S(t)$ is said to be unstable. The calculation of $\lambda_{\mathcal{P}}^\infty$ can be obtained with a single path by choosing $\tilde{\psi}_S(t) + \delta\tilde{\varphi}(t) = \tilde{\psi}_S(t + \delta t)$.

We have obtained the definition of \mathcal{P} -Lyapunov exponent in (7) by overcoming the three objections to the definition in (2). We now put this definition to the test. The approach taken to find the \mathcal{P} -Lyapunov exponent has been kinematic and it is expected to be valid for classical-statistical and quantum states. First we show its validity for classical-statistical states and its equivalence to the classical-mechanical Lyapunov exponent for several examples. Consider the classical unstable map $\Phi(x) = rx$ with $r > 1$, for which the classical-mechanical Lyapunov characteristic exponent is $\lambda_c(\mathbf{x}_0) = \ln r$. After n steps the classical density evolves to $\rho_n(x) = P^n \rho(x) = \rho(x/r^n)/r^n$. Take as initial system state a square-looking function $\tilde{\psi}_S(x, 0) = \sqrt{\rho_0(x)} = \sqrt{\Theta(x) - \Theta(x - b)}$ and Θ the Heaviside function. The distance between the system state and the reference state $\tilde{\psi}_R = \tilde{\psi}_S(0)$ is found to be $d_{\mathcal{P}} = 2 \arccos |r^{-n/2}|$. Its corresponding *divergence* function (8) ultimately diverges exponentially and the \mathcal{P} -Lyapunov exponent in (7) can be calculated to be

$$\lambda_{\mathcal{P}}^\infty [\tilde{\psi}_S(0)] = \ln(r)/2 = \lambda_c(\mathbf{x}_0)/2, \quad (9)$$

half the classical-mechanical Lyapunov exponent. There is then sensitivity to initial conditions for classical statistical states and they are classified as unstable in the same manner than using classical-mechanical Lyapunov exponents for all r . Figure 1(a) shows the convergence of $\lambda_{\mathcal{P}}^t$ to $\lambda_{\mathcal{P}}^\infty$ for different values of r .

A more sophisticated map is the r -adic transformation $\Phi(x) = rx \, (\text{mod}1)$ with $r > 1$, which is an *exact* transformation [6] (therefore *mixing*) with classical-mechanical Lyapunov exponent $\lambda_c(\mathbf{x}_0) = \ln r$. A necessary feature added to instability for *mixing* systems is boundedness that implies, as in the classical-mechanical trajectory case, that the distance between the system state and the reference state is saturated at the value $2 \arccos |\langle \psi_S \rangle \langle \psi_R \rangle|$, but before this saturation takes place the \mathcal{P} -Lyapunov exponent can be extracted to be arbitrarily close to $\ln(r)/2 = \lambda_c(\mathbf{x}_0)/2$ by choosing a sufficiently localized initial classical-statistical state. A classical transformation related to the r -adic map of interest for us in the later discussion of quantum states is the baker's map, a map of the unit square onto itself of the form

$$\Phi(x, y) = (2x - [2x], (y + [2y])/2) \quad (10)$$

where $[.]$ indicates integer part. This map is area-preserving and *mixing* with classical-mechanical Lyapunov exponent $\ln 2$. Following the same steps as in the r -adic map, we find the same result with $r = 2$.

We have obtained classical-statistical state sensitivity to initial conditions and instability for classical-mechanical unstable and *mixing* maps. Encouraged by these results we now proceed to study quantum systems. To test our definition of \mathcal{P} -Lyapunov exponent for quantum states we first choose simple analytic cases, the parabolic barrier and the harmonic oscillator. All states of the harmonic oscillator (see Figure 1(b) for a Gaussian function) are stable, $\lambda_{\mathcal{P}}^\infty = 0$. For the parabolic barrier, with potential $V(x) = -m\omega^2 x^2/2$, and classical-mechanical Lyapunov exponent $\lambda_c(\mathbf{x}_0) = \omega$ there are stable and unstable quantum states. The most stable ones are the eigenstates ϕ_α and in fact any discrete sum of eigenstates $\psi_S = \sum_n c_n \phi_n$ is stable. On the other hand, states that use the contin-

uous spectrum are unstable. For example, the distance between a Gaussian initial state on top of the barrier, $\tilde{\psi}_S(x) = \exp(-m\omega_0 x^2/2\hbar)$, and the reference state is of the form $2 \arccos |\left(\cosh^2 \omega t + (\omega/\omega_0 - \omega_0/\omega)^2 \sinh^2 \omega t\right)^{-1/4}|$. Its corresponding *divergence* function (8) ultimately diverges exponentially with time and the \mathcal{P} -Lyapunov exponent in (7) is found to be

$$\lambda_{\mathcal{P}}^\infty [\tilde{\psi}_S(0)] = \omega/2 = \lambda_c(\mathbf{x}_0)/2. \quad (11)$$

Therefore, in contrast to the starting definition (2), there is quantum state sensitivity to initial conditions and quantum unstable paths. Figure 1(b) shows the convergence of $\lambda_{\mathcal{P}}^t$ to the \mathcal{P} -Lyapunov exponent $\lambda_{\mathcal{P}}^\infty$ for two states with different values of ω .

We now consider the added complication of classically *mixing* systems for which we will use the classical baker map in (10). Quantization of a classical map is not unique and we consider two quantum baker maps to illustrate two different types of behaviour. First we understand the map as defined in configuration space, as did Mendes [11] for the Arnol'd cat map, for which a quantum theory can be defined by the unitary Floquet operator U such that $\tilde{\psi}_S(x, y) \rightarrow \tilde{\psi}'_S(x, y) = \tilde{\psi}_S(\Phi^{-1}(x, y)) = U\tilde{\psi}_S(x, y)$ with Φ in (10) and $\hat{p}_{x,y} = -i\hbar\nabla_{x,y}$ the momentum. For this quantum map the situation is analogous to that of classical-statistical states under the baker map and one then finds state sensitivity and unstable quantum paths in the same way. The second quantization procedure that we consider understands the classical baker map in position-momentum space and we adopt the Balazs-Voros-Saraceno [12,13] quantization procedure. The new characteristic that interests us is the discreteness of the spectrum. As we have already found for the parabolic barrier, it is possible to have stable states made of a discrete sum of eigenstates [15,14,16,17] even when localized onto classically unstable structures [18]. However, this does not pose a problem for the correspondence principle as for systems that appear classical to us the recurrence times of the quantum states are longer than the age of the Universe [19]. In typical numerical and experimental results the recurrence times due to the discreteness of the spectrum might be longer than that due to classical boundedness by the energy hypersurface. We relax

the mathematical convenience of considering asymptotic definitions and consider covered values for experimentally relevant times. Observe in Figure 1 that nonasymptotic values already give a classification of states by their sensitivity and instability for finite times. We now proceed to study the Balazs-Voros-Saraceno quantum map. Position and momentum are discretized $q_j = p_j = (j + 1/2)/N$ for $j = 0, \dots, N - 1$ with N even. The transformation between the position basis $\{|q_j\rangle\}$ and the momentum basis $\{|p_j\rangle\}$ is given by $(G_N)_{ij} = \langle p_i | q_j \rangle$ and the baker map is then defined as

$$\tilde{B} \equiv G_N^{-1} \begin{pmatrix} G_{N/2} & 0 \\ 0 & G_{N/2} \end{pmatrix}, \quad (12)$$

where the matrices $G_{N/2}$ map position kets on the lower (upper) half of the position interval to the lower (upper) part of the momentum interval and G_N^{-1} maps back to the position representation. We choose as initial quantum state $\tilde{\psi}_S(q_j) = \exp(-(q_0 - q_j)^2/2\alpha + ip_0 q_j/\alpha)$ with $\alpha = 10^4$ and $q_0 = p_0 = 0.003$. Figure 2(a) shows the finite-time \mathcal{P} -Lyapunov exponent for $N = 1800$ and times shorter than the bounded time $t_b \approx 8$ and it is found to be close to half the classical-mechanical Lyapunov exponent $\ln(2)/2$ as in the previous examples.

The notion of \mathcal{P} -Lyapunov exponent introduced in this paper can be measured in many types of experimental set-ups. It can be measured in optical filtering experiments by the different reduction of intensity of two nearby states. In molecular experiments the distance between the system state and the reference state can be obtained from the Fourier transform of the Franck-Condon spectrum. Very recently, Gardiner *et al.* [4] have proposed an ion trap set-up as a practical realization of a delta-kicked harmonic oscillator to measure the Peres [1] overlap $O(t) = |\langle \psi_S | \hat{U}_1^\dagger(t) \hat{U}_2(t) | \psi_S \rangle|^2$ with \hat{U}_1 and \hat{U}_2 two close unitary evolution operators to study the state sensitivity to changes in the Hamiltonian. We can reinterpret their results as sensitivity to initial conditions in the following manner. Consider the two nearby vectors $|\psi_S(t)\rangle = \hat{U}_1^{-1}(t) \hat{U}_2(t) |\psi_S(0)\rangle$ and $|\psi_S(t+dt)\rangle$. Their distances from the reference vector $|\psi_R\rangle = |\psi_S(0)\rangle$ are given in terms of the Peres overlap by $2 \arccos O(t)$. Figure 2(b) shows the *divergence* function for the two states of Fig.4(b) and (d) of [4], respectively. Figure 2(b)

also shows the \mathcal{P} -Lyapunov exponent and we find that one path is unstable with $\lambda_{\mathcal{P}} \approx 0.017$ and the other stable with $\lambda_{\mathcal{P}} \approx 0$.

The classification performed by the quantum \mathcal{P} -Lyapunov exponent will be in general different from the classical-mechanical one, but they must coincide in the classical limit. To see this first note that the Wigner representation or coherent state representation of the quantum state reduce to the classical Liouville density in the classical limit [2]. Moreover, the classification performed by the classical-statistical (Liouville) \mathcal{P} -Lyapunov exponent coincides with the one given by classical-mechanical Lyapunov exponents. To see this note that the distance between two classical densities given by (3) when the underlying trajectories obey $\mathbf{x}(t) = \mathbf{x}(0) \exp(\lambda_c t)$, with λ_c the classical-mechanical Lyapunov exponent, is obtained to be $d_{\mathcal{P}} [\tilde{\psi}_S, \tilde{\psi}_R] = \arccos(\exp(-\lambda_c t))$ and the classical Liouville \mathcal{P} -Lyapunov exponent reduces to $\lambda_{\mathcal{P}} [\tilde{\psi}_S(0)] = \lambda_c/2$. This property opens the possibility of studying in detail the classicalization of instability, most interestingly by the calculation of the quantum \mathcal{P} -Lyapunov exponent when adding classical or quantum noise and with increasing dimensionality of the system.

To conclude, a successful measure of quantum and classical-statistical state sensitivity to initial conditions and instability has been obtained. The classification given for quantum states reduces in the classical limit to that performed by classical-mechanical Lyapunov exponents. This classification has been studied in several examples, including recently proposed ion trap states.

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FIGURE CAPTIONS

Figure 1. Classification of states by their sensitivity to initial conditions as measured by the \mathcal{P} -Lyapunov exponent in (7) for (a) classical-statistical states under the unstable map $\Phi(x) = rx$ with $r = 2, 3$ and 5 converging to half the classical-mechanical Lyapunov exponent $\ln(r)/2$ and (b) for quantum states in the harmonic oscillator and the parabolic barrier with $\omega = 2$ and 5 converging to half the classical Lyapunov exponent $0, 1$ and 2.5 , respectively.

Figure 2. Classification of quantum states with discrete spectrum by their finite-time \mathcal{P} -Lyapunov exponent. Panel (a) shows the finite-time \mathcal{P} -Lyapunov exponent for the quantum baker map close to $\ln(2)/2$. The probability density is shown as an inset. Panel (b) shows the *divergence* function (8) for a state centered on a classically regular region and a state centered on a classically chaotic region of a delta-kicked harmonic oscillator, indicated by (1) and (2) respectively. The inset shows their corresponding finite-time \mathcal{P} -Lyapunov exponent that converges approximately to 0 and 0.017 . The data for (b) has been obtained from the experimental proposal of Gardiner *et al.* [4] on an ion trap set-up.

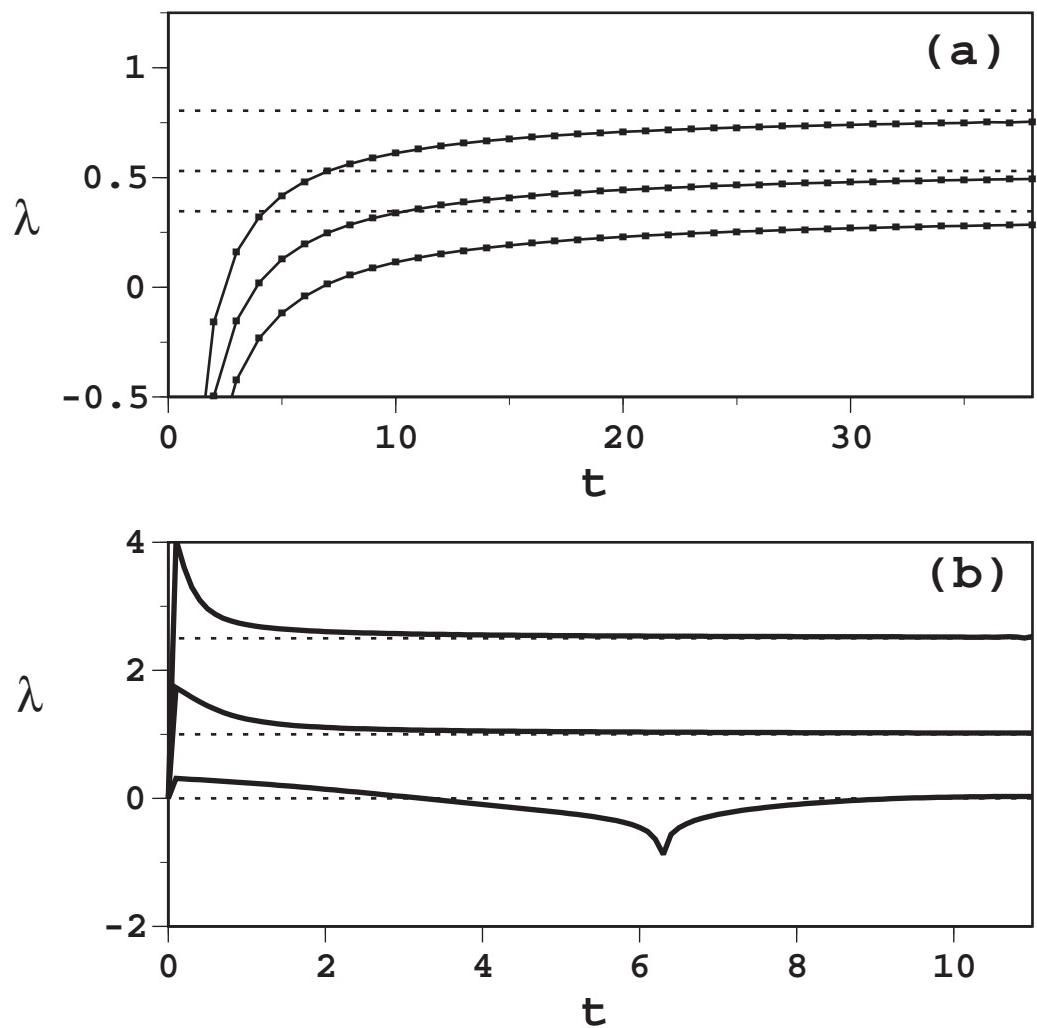


Figure 1.

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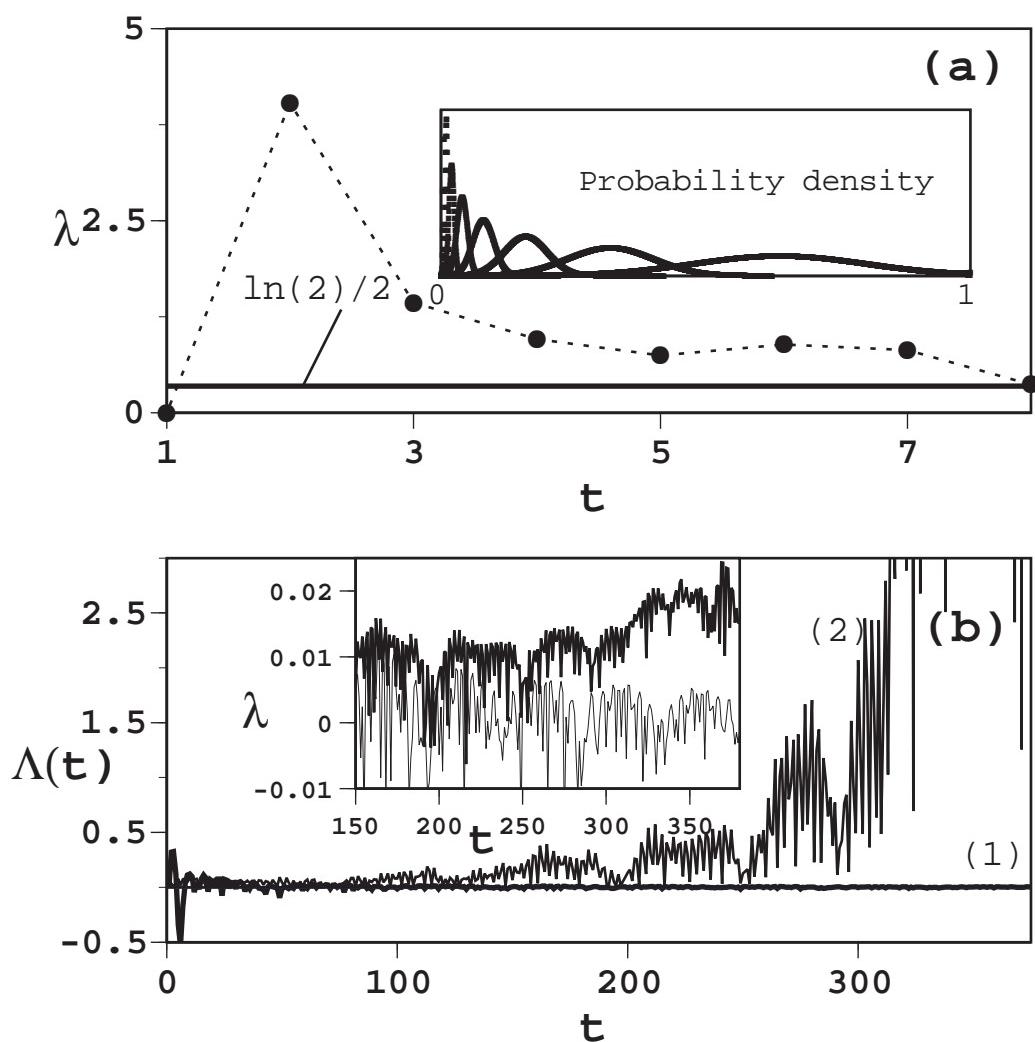


Figure 2.
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